Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Nuclear Instruments and Methods in Physics Research A 519 (2004) 53–62
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A
www.elsevier.com/locate/nima

New approaches for the validation of transfer maps using remainder-enhanced differential algebra

M. Berz[a,*], K. Makino[b]

[a] Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA
[b] Department of Physics, University of Illinois at Urbana-Champaign, 1110 W. Green Street, Urbana, IL 61801-3080, USA

Abstract

High-order transfer maps of particle systems play an important role in the design and optimization of particle optical systems, both for satisfying the basic design needs as well as for the correction of aberrations and non-linear effects, and the differential algebraic (DA) method has proved useful for this problem. Since the high-order maps represent an approximation of the motion, in particular in strongly nonlinear cases in which convergence of the maps may be slow, it is important to know the quality of the approximation. Recent work has shown that it is in principle possible to not only propagate the conventional differential algebraic high-order objects, but also adjoint remainder terms that rigorously account for any errors made by the approximation by the Taylor expansion over the domain of interest.

In this paper we describe various recent enhancements of the original method of computations with remainder bounds that allow the control of the errors made both by the integrator scheme and any possible inaccuracy of the description of the system.

Using suitable extensions of the DA and Taylor model operators used in the Schauder fixed point theorem formulation of the ODE problem leads to a very transparent approach for the calculation of enclosures for the intergration errors. Under the presence of a scheme for effective treatment of sparsity in the DA vectors, such as the method available in the code COSY INFINITY, the additional resources necessary for this algorithm are very modest.

PACS: 02.30.Hq; 02.30.Mv; 02.30.Sa; 02.60.Gf; 02.60.Lj; 05.45.−a; 29.27.−a; 41.85.−p

Keywords: Transfer map; Error verification; Remainder-enhanced differential algebra; Taylor model; Interval arithmetic; COSY INFINITY

1. Introduction

We begin with a recent enhancement of the original DA methods that allows to not only obtain transfer maps to high order, but at the same time and with very limited additional computational effort also determine fully rigorous bounds for the remainders in the Taylor expansion of a given order. The approach is based on utilizing the three differential algebraic (DA [1]) operations of addition, multiplication, derivation and their inverses on so-called Taylor model [2–4] objects for the direct solution of the Picard fixed point form of the differential equation. Employing

*Corresponding author.
E-mail addresses: berz@msu.edu (M. Berz), makino@uiuc.edu (K. Makino).

0168-9002/$ - see front matter
doi:10.1016/j.nima.2003.11.120

Schauder's theorem and compactness and convexity arguments for certain function spaces described by Taylor models, it is possible to construct verified integrators that perform a rigorous error analysis of their steps [5]. Compared to other verified integrators, the ones developed here avoid the so-called wrapping effect problem [6–8], which hampers conventional such approaches, and would otherwise prevent the treatment of typical beam physics problems.

One of the applications of the availability of maps with rigorous remainder bounds is the determination of optimal generators for symplectic tracking [9–11]. Besides the conventionally known four generators, there is an infinite family of others, all of which can be determined with DA methods. It is possible to identify those of the family that yield optimal symplectification in the sense of a metric that is invariant under symplectomorphisms. This assures that the generator is not only optimal for a given Poincare sections, but simultaneously for all others around the ring, and that it works as well for the millionth turn as it does for the first.

Using the rigorous remainder bounds of maps, it is possible to not only assure the existence of the generators locally, but to determine regions of phase space over which with certainty the map can be represented by a given generator. In practical examples it is found that as expected, the optimal generators maximize this region [11,12].

The methods are particularly useful for the study of systems where conventional symplectic tracking via kick approximations is not possible because the Hamiltonian cannot be decomposed into two explicitly solvable parts, as in all split-operator approaches. This is for example the case when the so-called kinematic correction is relevant, as in the case of the various accelerators and rings for neutrino machines. Symplectification can in this case be achieved with the use of generating functions; but because of the inherent strong nonlinearity, the use of optimal symplectification is of prime importance. Various examples of the performance of the methods for such machines are given in [11].

All the methods discussed here have been implemented within the DA environment of COSY INFINITY [13]. In order to facilitate interaction with other language environments, the COSY system has been ported to a language independent environment, which allows automatic code generation for use as F90 and C++ objects [4]. The advantage of the resulting tight and robust wrappers is that most of the inherent speed and efficiency of the original FORTRAN-based COSY tools is maintained, which has not been possible with native object oriented implementations.

2. Differential algebras

The differential algebraic approach [14–16] took the computation of Taylor maps

$$\vec{z}_f = \mathcal{M}(\vec{z}_i) \tag{1}$$

of dynamical systems from the customary third [17–20] or fifth order [21] all the way to arbitrary order in a unified and straightforward way. The Taylor maps have many applications, as many of the physical quantities that are encountered in practice are more or less directly connected to Taylor coefficients. Since its introduction, the method has been widely utilized in a large number of new map codes [13,22–28]

The basic idea behind the method is to bring the treatment of functions to the computer in a similar way as the treatment of numbers. In a strict sense, neither functions (for example, C^∞) nor numbers (for example, the reals R) can be treated on a computer, since neither of them can be represented with the finite amount of information that can be stored on computers. However, from the early days of computers we are used to dealing with numbers by extracting information deemed relevant, which in practice usually means the approximation by floating point numbers with finitely many digits. In a formal sense this is possible since for every one of the operations on real numbers, like addition and multiplication, we can craft an adjoint operation on the floating point numbers such that the following

diagram commutes:

$$\begin{array}{ccc} a,b\in R & \xrightarrow{T} & \bar{a},\bar{b}\in FP \\ \Big\downarrow * & & \Big\downarrow \circledast \\ a*b & \xrightarrow{T} & \bar{a}\circledast\bar{b} \end{array} \tag{2}$$

Of course, much to the chagrin of those doing numerics, in reality the diagrams commute only "approximately", which typically makes the errors grow over time.

The approximate character of these arguments can be removed by representing a real not by one floating point number, but rather by an interval of floating point numbers providing a rigorous upper and lower bound [6,8,29,30]. By rounding operations down for lower bounds and up for upper bounds, rigorous bounds can be found for sums and products, and adjoint operations can be made such that the above diagram commutes exactly. In practice, while always maintaining rigor, the method sometimes becomes rather pessimistic, as over time the intervals often have a tendency to grow.

Historically, the treatment of functions in numerics has been done based on the treatment of numbers; and as a result, virtually all classical numerical algorithms are based on the mere evaluation of functions at specific points. As a consequence, numerical methods for differentiation, which are so relevant for the computation of Taylor representations of the map (1), are very cumbersome and prone to inaccuracies because of cancellation of digits, and not useful in practice for our purposes.

The success of the DA methods is based on the observation that it is possible to extract more information about a function than its mere values. Indeed, considering the commuting diagram in Eq. (2), one can demand the operation T to be the extraction of the Taylor coefficients of a prespecified order n of the function. In mathematical terms, T is an equivalence relation, and the application of T corresponds to the transition from the function to the equivalence class comprising all those functions with identical Taylor expansion to order n. Since Taylor coefficients of order n for sums and products of functions as well as scalar products with reals can be computed from those of the summands and factors, it is clear that the diagram can be made to commute; indeed, except for the underlying inaccuracy of the floating point arithmetic, it will even commute exactly. In mathematical terms, this means that the set of equivalence classes of functions can be endowed with well-defined operations, leading to the so-called Truncated Power Series Algebra (TPSA) [14,15].

This fact was realized in the first paper on the subject [15], which led to a method to extract maps to any desired order from a computer algorithm that integrates orbits numerically. Similar to the need for algorithms within floating point arithmetic, the development of algorithms for functions followed, including methods to perform composition of functions, to invert them, to solve nonlinear systems explicitly, and to introduce the treatment of common elementary functions [31,32]. Very soon afterwards it became apparent [33,16] that this only represents a half-way point, and one should proceed beyond mere arithmetic operations on function spaces of addition and multiplication and consider their analytic operations of differentiation and integration. This resulted in the recognition of the underlying differential algebraic structure and its practical exploitation [1], based on the commuting diagrams for addition, multiplication, and differentiation and their inverses:

$$\begin{array}{ccc} f,g & \xrightarrow{T} & F,G \\ +,-,\cdot,/\ \Big\downarrow & & \Big\downarrow \oplus,\ominus,\odot,\oslash \\ f\overset{+}{-}g,f\overset{\cdot}{/}g & \xrightarrow{T} & F\overset{\oplus}{\ominus}G,F\overset{\odot}{\oslash}G \end{array} \qquad \begin{array}{ccc} f & \xrightarrow{T} & F \\ \partial,\partial^{-1}\ \Big\downarrow & & \Big\downarrow \partial_{\bigcirc},\partial_{\bigcirc}^{-1} \\ \partial f,\partial^{-1}f & \xrightarrow{T} & \partial_{\bigcirc}F,\partial_{\bigcirc}^{-1}F \end{array} \tag{3}$$

In passing we note that in order to avoid loss of order, in practice the derivations have the form

$\partial = h \cdot \mathrm{d}/\mathrm{d}x_i$, where h is a function with $h(0) = 0$. As a first consequence, it allowed to construct integration techniques to any order that for a given accuracy demand are substantially faster than conventional methods [32]. Subsequently, it was realized that the differential algebraic operations are useful for a whole variety of other questions connected to the analytic properties of the transfer map [31]. It was possible to determine arbitrary order generating function representations of maps [34,32]; factorizations into Lie operators [35] could be carried out for the first time to arbitrary order [32]; normal form methods [36,37] could be performed to arbitrary order [38,32]. And last but not least, the complicated PDEs for the fields and potentials stemming from the representation of Maxwell's equations in particle optical coordinates could be solved to any order in finitely many steps [1].

Of course the question of what constitutes "information deemed relevant" for functions does not necessarily have a unique answer. Formula manipulators, for example, attack the problem from a different perspective by attempting to algebraically express functions in terms of certain elementary functions linked by algebraic operations and composition. In practice the Achilles heel of this approach is the complexity that such representations can take after only a few operations. But compared to the mere Taylor expansion, they have the advantage of rigorously representing the function under consideration. In the following we will show how such rigor can be maintained without the computational expense of formula manipulation by a suitable augmentation of the Taylor approach.

3. Remainder-enhanced differential algebras

Compared to techniques of formula manipulation and to other rigorous mathematical efforts on computers, the Taylor DA methods do not make any statements about the remainder of Taylor's formula. By extending the theory, it is possible to obtain rigorous bounds for the remainder terms. In this endeavour, we demand to be fully mathematically rigorous in that no approximations are allowed. All this is achieved by keeping the idea of providing commuting diagrams for elementary operations; however, the objects on which these operations are to be carried out are not mere truncated Taylor series any more, but rather new objects called Taylor models [2,3].

Furthermore, in order to keep the mathematical rigor for the solution of the differential equations defining the maps of the systems, we had to derive a new method to perform integration [5]. As in many other automated approaches for integration of functions and differential equations on computers, we utilize differential algebraic techniques for this purpose. While in the conventional computation of Taylor maps, in principle also conventional integrators can be used, this is not the case here, and one is more or less forced to develop new techniques. Our method relies on an inclusion of the remainder term of a Taylor expansion in an interval. However, to quell misunderstandings from the beginning, it is important to note that our approach is not equivalent to interval methods that have been applied extensively for many types of verified calculations [6,8,29,30]. Our method provides remainder bounds with an accuracy that does not scale merely linear with the domain interval, but rather as a high power of the domain interval; this feature is essential if high accuracy is required over an extended range of arguments, as is the case with the transfer map. Furthermore, it alleviates the so-called dependency problem [39], which among other things entails that extended conventional interval computations sometimes "blow up" and yield rather pessimistic and sometimes even useless bounds.

We begin with the definition of a Taylor model. Let f be $C^{(n+1)}$ on $D_f \subset R^v$, and $\vec{B} = [\vec{a}, \vec{b}] \subset D_f$ an interval box containing the point $\vec{x}_0$. Let T be the Taylor polynomial of f around $\vec{x}_0$. We call the interval I an nth order remainder bound of f on $\vec{B}$ if

$$f(\vec{x}) - T(\vec{x}) \in I, \quad \forall \vec{x} \in \vec{B}.$$

In this case, we call the pair (T, I) an nth-order Taylor model of f. It is clear that a given function f can have many different Taylor models, as with (T, I), also $(T, \bar{I})$ with $\bar{I} \supset I$ is a Taylor model. Furthermore, we see that low-order polynomials

have trivial remainder bounds; since every polynomial of order not exceeding n agrees with its nth order Taylor polynomial, the interval $[0,0]$ is a remainder bound. For practical purposes, it is important that if the original interval box $\vec{B}$ decreases in size, then according to the various formulas of the Taylor remainder, the remainder bounds can decrease in size with a power of $n+1$ and hence will become small quickly. In particular, this entails that the knowledge of a good Taylor model of a function on an interval box $\vec{B}$ allows a rather accurate estimate of the range of the function.

Now we define arithmetic operations on Taylor models. In this case, the operation "T" that turns a function into its Taylor polynomial has to be replaced by the inclusion operation $\subset$. So we must craft new adjoint operations on Taylor models that make the diagram

$$\begin{array}{ccc} f,g\in C^{n+1} & \xrightarrow{\ \subset\ } & (T_f,I_f),(T_g,I_g) \\ \Big\downarrow * & & \Big\downarrow \circledast \\ f*g & \xrightarrow{\ \subset\ } & (T_f,I_f)\circledast(T_g,I_g) \end{array}$$

commute in a similar way as in the case of the differential algebra on truncated power series in Eq. (3).

Let (T_f,I_f) and (T_g,I_g) be nth-order Taylor models of the functions f and g on $\vec{B}$. Clearly, the Taylor polynomial of $(f+g)$ is simply T_f+T_g; on the other hand, we know that on $\vec{B}$, $f(\vec{x})\in T_f(\vec{x})+I_f$ and $g(\vec{x})\in T_g(\vec{x})+I_g$. Then obviously,

$$(f+g)(\vec{x})\in(T_f+T_g)(\vec{x})+(I_f+I_g)\quad\forall\vec{x}\in\vec{B},$$

and so (T_f+T_g,I_f+I_g) is a Taylor model for $(f+g)$ on $\vec{B}$. And for practical purposes, it is also important to note that if I_f, I_g are "fine of order $\vec{B}^{n+1}$", i.e. their size scales with the size of $\vec{B}$ to the $(n+1)$st power, so is $I_{f+g}=I_f+I_g$. In the same way we see that (T_f-T_g,I_f-I_g) is a Taylor model for $(f-g)$. So by simply defining

$$(T_f,I_f)\oplus(T_g,I_g)=(T_f+T_g,I_f+I_g),$$

we are able to close the commuting diagram for addition.

The nth-order Taylor polynomial $T_{f\cdot g}$ of $f\cdot g$ can be obtained by multiplication of T_f and T_g and subtraction of the polynomial $\bar{T}_{f\cdot g}$ consisting of the terms whose order exceeds n. For any $\vec{x}\in\vec{B}$, there are values $e_f\in I_f$ and $e_g\in I_g$ such that $f(\vec{x})=T_f(\vec{x})+e_f$ and $g(\vec{x})=T_g(\vec{x})+e_g$. So we obtain

$$\begin{aligned}&(f\cdot g)(\vec{x})\\&\quad=(T_f(\vec{x})+e_f)\cdot(T_g(\vec{x})+e_g),\\&\quad=T_f(\vec{x})\cdot T_g(\vec{x})+T_f(\vec{x})\cdot e_g+T_g(\vec{x})\cdot e_f+e_f\cdot e_g,\\&\quad=T_{f\cdot g}(\vec{x})+\{\bar{T}_{f\cdot g}(\vec{x})+T_f(\vec{x})\cdot e_g+T_g(\vec{x})\cdot e_f\\&\qquad+e_f\cdot e_g\}.\end{aligned}$$

The first term is the nth-order Taylor polynomial of $f\cdot g$. The term in curly brackets describes the behavior of the remainder; it is a polynomial in the $v+2$ variables $(\vec{x},e_f,e_g)\in\vec{B}\times I_f\times I_g$ and is denoted by $R(\vec{x},e_f,e_g)$. So by bounding $R(\vec{x},e_f,e_g)$ [2,3] with an interval I_R, we are able close the diagram with the definition

$$(T_f,I_f)\odot(T_g,I_g)=(T_{f\cdot g},I_R).$$

We note that the necessary computation of $T_{f\cdot g}$ from T_f and T_g is of course the standard multiplication within TPSA.

The operations $\oplus$ and $\odot$ for Taylor models, in themselves, are already useful for several problems in Beam Physics, in particular for the notoriously difficult bounding of approximate invariants of non-linear motion [40]. Besides them, there are a variety of other operations that have to be ported to the Taylor models, especially the intrinsic functions, the composition of functions, and several operations derived from these [2,3], and a complete set of standard functions on computers was implemented in COSY INFINITY [3,4].

Before proceeding further, let us investigate the inverse derivation operation $\partial_{\bigcirc}^{-1}$ on Taylor models. Given an nth-order Taylor model (T_f,I_f) of a function f, we can determine a Taylor model for the indefinite integral $\partial_i^{-1}f=\int f\,\mathrm{d}x_i'$ with respect to variable i. The Taylor polynomial part is obviously just given by $\int T_{f,n-1}\,\mathrm{d}x_i'$, where $T_{f,n-1}$ is the $(n-1)$th-order Taylor polynomial, and a remainder bound can be obtained as $(B(T_f-T_{f,n-1})+I_f)\cdot B(x_i)$, where $B(x_i)$ is an interval bound for the variable x_i obtained from the range of definition of x_i, and $B(T_f-T_{f,n-1})$ is a bound

for the part of T_f that is of exact order n. We thus define the operator $\partial_{\bigcirc,i}^{-1}$ on the space of Taylor models as

$$\partial_{\bigcirc,i}^{-1}(T_f, I_f) = \left(\int T_{f,n-1}\, \mathrm{d}x_i,\ (B(T_f - T_{f,n-1}) + I_f) \times \cdot B(x_i) \right).$$

The introduction of the operator $\partial_{\bigcirc,i}$ is also possible, however at an additional effort, since from the knowledge of a remainder bound of a function, no conclusions can be drawn regarding a remainder bound for its derivative.

4. Computation of remainder bounds for flows of differential equations

We now establish a Taylor model for the transfer map $\mathscr{M}(\vec{r}_0, t)$, and in particular a rigorous bound for the remainder term of the flow of the differential equation describing the motion over a domain $[\vec{r}_{01}, \vec{r}_{02}] \times [t_0, t_1]$. As pointed out before, this need precludes us from the direct use of conventional numerical integrators, as they cannot provide rigorous bounds for the integration error but only approximate estimates. Rather, we have to start from scratch from the foundations of the theory of differential equations [5].

We use Taylor models for the solution of the initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{r}(t) = \vec{F}(\vec{r}(t), t), \quad \vec{r}(t_0) = \vec{r}_0,$$

where $\vec{F}$ is continuous and bounded. We are interested in both the case of a point initial condition $\vec{r}_0$, and the case in which the initial condition $\vec{r}_0$ is a variable. In the latter case, our interest is in the flow of the ODE

$$\vec{r}(t) = \mathscr{M}(\vec{r}_0, t),$$

describing the values of final coordinates in terms of initial coordinates and time. The solutions should be fully rigorous for all initial conditions $\vec{r}_0$ and times t that satisfy

$$\vec{r}_0 \in [\vec{r}_{01}, \vec{r}_{02}], \quad t \in [t_0, t_1].$$

In particular, $\vec{r}_0$ itself may be a Taylor model, as long as its range is known to lie in $[\vec{r}_{01}, \vec{r}_{02}]$.

As is commonly done, we re-write the ODE as an integral equation

$$\vec{r}(t) = \vec{r}_0 + \int_{t_0}^{t} \vec{F}(\vec{r}(t'), t')\, \mathrm{d}t',$$

and introduce the operator $A : \vec{C}^0[t_0, t_1] \to \vec{C}^0[t_0, t_1]$ on the space of continuous functions from $[t_0, t_1]$ to R^v via

$$A(\vec{f})(t) = \vec{r}_0 + \int_{t_0}^{t} \vec{F}(\vec{f}(t'), t')\, \mathrm{d}t'.$$

Then the problem of finding a solution to the ODE is transformed to a fixed-point problem on the space of continuous functions

$$\vec{r} = A(\vec{r}).$$

We apply Schauder's fixed point theorem to rigorously obtain a Taylor model for the flow.

Theorem (Schauder). *Let A be a continuous operator on the Banach Space X. Let $M \subset X$ be compact and convex, and let $A(M) \subset M$. Then A has a fixed point in M, i.e. there is an $\vec{r} \in M$ such that $A(\vec{r}) = \vec{r}$.*

In our specific case, $X = \vec{C}^0[t_0, t_1]$, the Banach space of continuous functions on $[t_0, t_1]$, equipped with the maximum norm, and the integral operator A is continuous on X. The process to apply Schauder's theorem consists of the following steps:

- Determine a family Y of subsets of X, the Schauder candidate sets. Each set in Y should be compact and convex, it should be contained in a suitable Taylor model, and its image under A should be in Y.
- Using differential algebraic (DA) methods on Taylor models, determine an initial set $M_0 \in Y$ that satisfies the inclusion property $A(M_0) \subset M_0$. Then all requirements of Schauder's theorem are satisfied, and M_0 contains a solution.
- Iteratively generate the sequence $M_i = A(M_{i-1})$ for $i = 1, 2, 3, \ldots,$. Each M_i also satisfies $A(M_i) \subset M_i$, and we have

$M_1 \supset M_2 \supset \cdots$. We continue the refinement iteration until the size stabilizes sufficiently.

- If integration over extended time intervals is needed, as is commonly the case, split the interval into sufficiently small pieces and successively apply the above technique.

The first step can be satisfied by the mathematical properties of Taylor models and the right hand side of the ODE, $\vec{F}$. For details of these rather mathematical matters, we refer the reader to [5]. The second step can be simplified greatly by choosing the optimal polynomial $\vec{P}$ for the initial set M_0; choose the n-th order flow $\mathscr{M}_n(\vec{r}_0, t)$ for $\vec{P}$ using the DA fixed point algorithm [1]. Since $\mathscr{M}_n(\vec{r}_0, t)$ is the DA fixed point, the remaining task for the inclusion requirement and the refinement iteration boils down to a mere comparison task of the two intervals involved, which is computationally straightforward.

The method turned out to be extremely successful for validated initial value problems [41,42]. As mentioned earlier, the interval method is prone to blowup, making mere interval solutions difficult in practice. In the case of multidimensional systems, a further source of overestimation arises from the need of geometric repackaging of the solution at each integration time step, called "wrapping effect" [6–8]. Fig. 1 illustrates the evolving wrapping effect in a harmonic oscillator, an error which grows exponentially unless controlled. This phenomenon makes the conventional interval based integration schemes difficult to obtain verified solutions for any practical problems [8,43]. In addition to the fact that remainder bounds in Taylor models are sharp, our scheme allows the initial condition $\vec{r}_0$ to be variables and thus represents the current flow not by an interval, but by a Taylor model in the initial conditions; this helps to control the wrapping effect optimally. We illustrate this effect with an example frequently used in the study of ODEs [8], the Volterra equations.

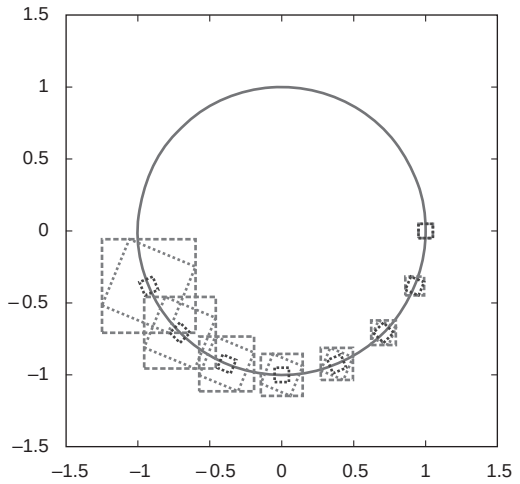

Fig. 1. The wrapping effect occurring in a harmonic oscillator.

Specifically, the problem is to solve the ODE

$$\frac{dx_1}{dt} = 2x_1(1 - x_2), \quad \frac{dx_2}{dt} = -x_2(1 - x_1)$$

with the initial condition domain interval box around $(1, 3)$ [44]. It can be shown that the solution trajectory forms a closed orbit for a point initial condition if both $x_{1\text{ini}}$ and $x_{2\text{ini}}$ are positive. Thus the solution trajectories with the initial condition interval box around $(1, 3)$ should form a band, and an effective verified integration scheme should provide a solution trajectory band without much inflation of the band width. We compared our Taylor model based verified integrator and AWA [45], a very popular verified integrator, for the initial condition interval box

$$x_{1\text{ini}} \in 1 + [-0.05, 0.05], \quad x_{2\text{ini}} \in 3 + [-0.05, 0.05].$$

While AWA suffers from the wrapping effect and cannot proceed beyond about one half of the cycle, the Taylor model-based integrator completes the cycle even without any visible inflation of the band width. The developing elongation of the solution region in Fig. 2 along the trajectory is due to the different cycle periods of closed orbits.

5. Validated maps of particle optical systems

In the following we apply the validated integrator to the computation of some verified transfer maps in particle optics. In both cases, the motion is split into small sub-pieces, as is commonly done in numerical integration, and over the sub-piece expansion in time is performed. In the first

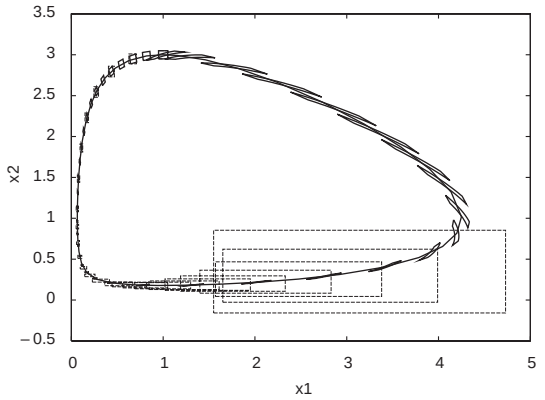

Fig. 2. Solution regions of the Volterra equations starting from the initial condition interval box $x_{1\mathrm{ini}} \in 1 + [-0.05, 0.05]$, $x_{2\mathrm{ini}} \in 3 + [-0.05, 0.05]$ by Taylor models (solid regions) and AWA (dashed boxes).

example we analyze the motion of a charged particle in a dipole magnet with constant magnetic field over an extended phase space. Since the motion in the dipole can be solved analytically based on simple geometrical arguments related to intersections of circles and straight lines, this problem represents a useful check of the practical validity of the remainder bounds. For our example, we chose a magnet with a deflection radius $R = 1$ m. The integration was carried out over a deflection angle of 36° with a fixed step size of 4°. The four initial conditions for horizontal position x, horizontal relative momentum $a = p_x/p_0$, vertical position y, and vertical relative momentum $b = p_y/p_0$ all lie within the interval $[-0.02, 0.02]$, and the Taylor polynomial describing the dependence of the four final coordinate values on the four initial coordinate values was determined. The order in time and initial conditions was chosen to be 12, so that the expansion in time could be carried over a sufficiently large interval. In the present implementation, for technical reasons this also entails that the expansion in the phase space variables is carried to the same order, although it is observed that the orders beyond 7 contribute only insignificantly. The actual step size was estimated so as to ascertain an overall accuracy below 10^{-9}; since no automatic step size control was utilized, the estimate proved conservative and the actual resulting remainder bounds were somewhat smaller; they were found to be

$$[-0.4496880372277553\mathrm{E}-09,\ +0.3888593417126594\mathrm{E}-09]$$

$$[-0.1301070602141642\mathrm{E}-09,\ +0.1337099965985420\mathrm{E}-09]$$

$$[-0.3417079805637740\mathrm{E}-10,\ +0.3417079805637740\mathrm{E}-10]$$

$$[-0.0000000000000000\mathrm{E}+00,\ +0.0000000000000000\mathrm{E}+00]$$

for the x, a, y and b coordinates in common particle optical terminology [1].

The resulting Taylor polynomials describing the dependence of final on initial coordinates were compared with the corresponding dipole transfer map obtained by the standard DA method, and agreement was found. Furthermore, the final coordinates for a large collection of rays were studied to compare between the geometric determination and the Taylor polynomial computation, and the difference was within the calculated remainder bounds.

The next example is to verify the mapping functions for a more complicated beam optics system, a typical FODO cell of an accelerator lattice. The cell is set up consisting of the following sequence of elements: drift, defocusing quadrupole superimposed with a sextupole, drift, dipole, drift, defocusing quadrupole superimposed with a sextupole, and drift. The defocusing quadrupoles have the same strength $k = -0.0085$, and the sextupole strength is $h = 0.06$. The lengths are 1 m for the drifts and 0.5 m for the magnets; the dipole's curvature radius is 2.5 m and the reference particle is a proton with an energy of 1 MeV.

We performed a verified integration through the cell using the 17th-order Taylor models on the relatively large initial condition domain interval box of $[-0.1, 0.1]$ in each direction of phase space. An automatic step size control scheme was applied to suppress the growth of the remainder bound optimally. Integration of the system yielded a Taylor model containing the true solution of the corresponding differential equations. In the

following we list the first ten terms of the Taylor model containing the x-component of the flow, which is the function mapping the initial conditions x_0, a_0, y_0, and b_0 to the x position at the end of the cell.

```
RDA VARIABLE: NO=17, NV=4
I  COEFFICIENT             ORDER EXPONENTS
1  0.1398389113940111      1     1  0  0  0
2  0.1038317686361456      1     0  1  0  0
3  -.2447944264979660E-01  2     2  0  0  0
4  -.1183394850192213E-01  2     1  1  0  0
5  -.2119694344941219E-02  2     0  2  0  0
6  0.2361409770673162E-01  2     0  0  2  0
7  0.1212766097410308E-01  2     0  0  1  1
8  0.2185093364668458E-02  2     0  0  0  2
9  0.9944830763540945E-03  3     3  0  0  0
10 0.8715481705011164E-03  3     2  1  0  0
```

with the remainder bound as follows.

```
[−.2157121190249145E − 012,
  0.2178948979195422E − 012]
```

It should be noted that the Taylor model encloses the flow with a relative overestimation of better than 10^{-10}, which shows the ability of the Taylor model approach to integrate over the length of the entire FODO cell with a large size domain for the initial condition.

Acknowledgements

We would like to thank Jens Hoefkens and Béla Erdélyi for the calculation of the last example in this paper. We are also thankful for various useful comments by two anonymous referees. The work was supported in part by the US Department of Energy, an Alfred P. Sloan Fellowship and in part by the Illinois Consortium for Accelerator Research and the National Science Foundation.

References

[1] M. Berz, Modern Map Methods in Particle Beam Physics, Academic Press, San Diego, 1999.
[2] K. Makino, M. Berz, Remainder differential algebras and their applications, in: M. Berz, C. Bischof, G. Corliss, A. Griewank (Eds.), Computational Differentiation: Techniques, Applications, and Tools, SIAM, Philadelphia, PA, 1996, pp. 63–74.
[3] K. Makino, Rigorous analysis of nonlinear motion in particle accelerators, Ph.D. Thesis, Michigan State University, East Lansing, MI, USA, 1998, also MSUCL-1093.
[4] M. Berz, J. Hoefkens, K. Makino, COSY INFINITY Version 8.1-programming manual, Technical Report MSUHEP-20703, Department of Physics and Astronomy, Michigan State University, East Lansing, MI, 2001, see also http://cosy.pa.msu.edu.
[5] M. Berz, K. Makino, Reliable Comput. 4 (4) (1998) 361.
[6] R.E. Moore, Interval Analysis, Prentice-Hall, Englewood Cliffs, NJ, 1966.
[7] F. Krückeberg, Ordinary differential equations, in: E. Hansen (Ed.), Topics in Interval Analysis, Clarendon Press, Oxford, 1969, pp. 91–97.
[8] R.E. Moore, Methods and Applications of Interval Analysis, SIAM, Philadelphia, PA, 1979.
[9] B. Erdélyi, M. Berz, Local theory and applications of extended generating functions, Int. J. Pure Appl. Math., in press.
[10] B. Erdélyi, M. Berz, Phys. Rev. Lett. 87 (11) (2001) 114302.
[11] B. Erdélyi, Symplectic approximation of hamiltonian flows and accurate simulation of fringe field effects, Ph.D. Thesis, Michigan State University, East Lansing, MI, USA, 2001.
[12] J. Hoefkens, Verified methods for differential algebraic equations, Ph.D. Thesis, Michigan State University, East Lansing, MI, USA, 2001.
[13] M. Berz, K. Makino, COSY INFINITY Version 8.1—user's guide and reference manual, Technical Report MSUHEP-20704, Department of Physics and Astronomy, Michigan State University, East Lansing, MI, 2001; see also http://cosy.pa.msu.edu.
[14] M. Berz, The new method of TPSA algebra for the description of beam dynamics to high orders, Technical Report AT-6:ATN-86-16, Los Alamos National Laboratory, 1986.
[15] M. Berz, Nucl. Instr. and Meth. A 258 (1987) 431.
[16] M. Berz, Part. Accel. 24 (1989) 109.
[17] K.L. Brown, The ion optical program TRANSPORT, Technical Report 91, SLAC, 1979.
[18] H. Wollnik, J. Brezina, M. Berz, Nucl. Instr. and Meth. A 258 (1987) 408.
[19] T. Matsuo, H. Matsuda, Mass Spectrom. 24 (1976).
[20] A.J. Dragt, L.M. Healy, F. Neri, R. Ryne, IEEE Trans. Nucl. Sci. NS 3 (5) (1985) 2311.
[21] M. Berz, H.C. Hofmann, H. Wollnik, Nucl. Instr. and Meth. A 258 (1987) 402.
[22] L. Michelotti, MXYZTPLK: A practical, user friendly C++ implementation of differential algebra, Technical report, Fermilab, 1990.
[23] W.G. Davis, S.R. Douglas, G.D. Pusch, G.E. Lee-Whiting, The Chalk River differential algebra code DACYC and the role of differential and Lie algebras in understanding the orbit dynamics in cyclotrons, in: M. Berz, S. Martin, K. Ziegler (Eds.), Proceedings of the

Workshop on Nonlinear Effects in Accelerators, IOP Publishing, London, 1993.
[24] J. van Zeijts, F. Neri, The arbitrary order design code TLIE 1.0, in: M. Berz, S. Martin, K. Ziegler (Eds.), Proceedings of the Workshop on Nonlinear Effects in Accelerators, IOP Publishing, London, 1993.
[25] J. van Zeijts, New features in the design code TLIE, in: Third Computational Accelerator Physics Conference, New York, AIP Conference Proceedings, Vol. 297, 1993, p. 285.
[26] Y. Yan, C.-Y. Yan, ZLIB, a numerical library for differential algebra, Technical Report 300, SSCL, 1990.
[27] Y. Yan, ZLIB and related programs for beam dynamics studies, in: Third Computational Accelerator Physics Conference, New York, AIP Conference Proceedings, Vol. 297, 1993, p. 279.
[28] F.C. Iselin, The CLASSIC project. in: Fourth Computational Accelerator Physics Conference, New York, AIP Conference Proceedings, Vol. 391, 1997, p. 325.
[29] U.W. Kulisch, W.F. Miranker, Computer Arithmetic in Theory and Practice, Academic Press, New York, 1981.
[30] G. Alefeld, J. Herzberger, Introduction to Interval Computations, Academic Press, New York, 1983.
[31] M. Berz, Differential algebraic techniques, in: M. Tigner, A. Chao (Eds.), Handbook of Accelerator Physics and Engineering, World Scientific, New York, 1999.
[32] M. Berz, High-Order computation and normal form analysis of repetitive systems, in: M. Month, (Ed.), Physics of Particle Accelerators, Vol. 249, American Institute of Physics, New York, 1991, p. 456.
[33] M. Berz, Differential algebraic description of beam dynamics to very high orders, Technical Report SSC-152, SSC Central Design Group, Berkeley, CA, 1988.
[34] M. Berz, Symplectic tracking in circular accelerators with high order maps, in: Nonlinear Problems in Future Particle Accelerators, World Scientific, New York, 1991, p. 288.
[35] A.J. Dragt, J.M. Finn, J. Math. Phys. 17 (1976) 2215.
[36] A.J. Dragt, J.M. Finn, J. Math. Phys. 20 (12) (1979) 2649.
[37] A. Bazzani, Celestial Mech. 42 (1988) 107.
[38] E. Forest, M. Berz, J. Irwin, Part. Accel. 24 (1989) 91.
[39] K. Makino, M. Berz, Reliable Comput. 5 (1) (1999) 3.
[40] M. Berz, G. Hoffstätter, Interval Comput. 2 (1994) 68.
[41] M. Berz, K. Makino, J. Hoefkens, Nonlinear Anal. 47 (2001) 179.
[42] J. Hoefkens, M. Berz, K. Makino, Reliable Computing 9 (1) (2003) 21.
[43] R.J. Lohner, Einschliessung der Losung gewohnlicher Anfangs- und Randwertaufgaben und Anwendungen, Dissertation, Fakultat fur Mathematik, Universitat Karlsruhe, 1988.
[44] W.F. Ames, E. Adams, Monotonically convergent numerical two-sided bounds for a differential birth and death process, in: K. Nickel (Ed.), Interval Mathematics, Lecture Notes in Computer Science, Vol. 29, Springer, Berlin, New York, 1975, pp. 135–140.
[45] R.J. Lohner, Awa-software for the computation of guaranteed bounds for solutions of ordinary initial value problems. ftp://ftp.iam.uni-karlsruhe.de/pub/awa/